Applied Mathematical Modelling 36 (2012) 3813–3825

Contents lists available at SciVerse ScienceDirect

Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

Mathematical modelling and optimisation of a waste water treatment plant by combined oxygen electrode and biological waste water treatment model

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ARTICLE INFO

Article history:
Received 4 February 2011
Received in revised form 13 October 2011
Accepted 2 November 2011
Available online 15 November 2011

Keywords:
Mathematical modelling
Waste water treatment
Oxygen electrode
Process optimization

ABSTRACT

Structured mathematical models of oxygen electrode and biological waste water treatment were combined to optimise the position of electrode in the bioreactor. Parameters sensibility testing of mathematical model has shown that the model was most sensitive to the change of these parameters (in decreasing order of significance): oxygen consumption per unit of BOD_5, specific consumption rate of adsorbed BOD_5, volumetric coefficient of oxygen transfer rate (k_La), and waste water inflow. Two positions of electrode were tested: in the bioreactor and in the bioreactors syphon outlet shaft. Results obtained for the exchange of the oxic/anoxic phase and sludge recycling plant indicated that a reduction of electrical power for the aeration could be achieved if O_2 electrode is placed in the bioreactor tank, compared to position in outlet shaft. Better positioning of electrode has resulted in shortening of the oxic/anoxic cycle by 13% and the daily working time of aerators for 0.5 h per day, respectively. In the same time, the number of oxic/anoxic cycles per day was increased by 29%. In addition, results obtained by mathematical modelling indicated no debasement of chemical composition in out coming purified water if new position will be used.

1. Introduction

Global growth of human population and industrial development lead to daily increase of water consumption, with consecutive increase of waste water and solid waste. Social importance of water management has resulted in legal regulations targeted to optimise the outlet concentrations from waste water treatment plants. Large municipal waste water treatment plants are mostly constructed as a "channel" type or as a "closed loop type". Channel type of bioreactor could be represented as:

–Plug flow with or without axial dispersion [1],

–Ideally mixed tank in series with or without back-mixing [2–4]. One of the most common procedures applied in municipal waste water treatment plants (WWTP) is the aerobic biological processing with active sludge recycling and repeating nitrification and de-nitrification cycles (oxic/anoxic/anaerobic phases) performed in closed loop type of bioreactors called "oxidation ditches". Closed loop bioreactors (circulating flow reactors) applied in the waste water treatment plant are constructed with intention to be "well mixed" tanks.

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doi:10.1016/j.apm.2011.11.028

Nomenclature

ASM	activated sludge model
$\mathrm{BOD}_{5,\mathrm{in}}$	input concentration of BOD_5 [mg dm^{-3}]
$\mathrm{BOD}_{5,\mathrm{amax}}$	maximum possible amount of adsorbed BOD_5 calculated from the weight of the biomass [mg dm^{-3}]
C_f	oxygen concentration in laminar layer around electrode [mg dm^{-3}]
C_g	oxygen concentration in electrolyte gel of electrode [mg dm^{-3}]
C_m	oxygen concentration in membrane of oxygen electrode [mg dm^{-3}]
$C(\mathrm{O}_2)_{,\mathrm{bmax}}$	saturation constant for O_2 in wastewater on bottom of the bioreactor [mg dm^{-3}]
$C(\mathrm{O}_2)_{,\mathrm{tmax}}$	saturation constant for O_2 in wastewater on top of the bioreactor [mg dm^{-3}]
D	dilution rate [s^{-1}]
DO	dissolved oxygen [mg s^{-1}]
F	waste water flow [dm^3 s^{-1}]
F_r	recirculation flow [dm^3 s^{-1}]
k	$k_L a$ for aerobic phase [s^{-1}]
K_{ads}	saturation constant for adsorbed BOD_5 [mg (mg^{-1} dm^{-3})]
$Ka\mathrm{O}_2$	saturation constant for O_2, for autotrophic biomass [mg dm^{-3}]
$Kh\mathrm{O}_2$	saturation constant for O_2, for heterotrophic biomass [mg dm^{-3}]
$Ki\mathrm{O}_2$	inhibition constant for O_2 [mg dm^{-3}]
K_{NH_4}	saturation constant for NH_4^+ [mg dm^{-3}]
K_{NO_2}	saturation constant for NO_2^- [mg dm^{-3}]
K_{NO_3}	saturation constant for NO_3^- [mg dm^{-3}]
Ks	saturation constant for BOD_5 [mg dm^{-3}]
k_{STO}	specific adsorption rate for BOD_5 [kg (kg^{-1} s^{-1})]
$\mathrm{NH}_{4,\mathrm{in}}$	input concentration of NH_4^+ [mg dm^{-3}]
$\mathrm{NO}_{2,\mathrm{in}}$	input concentration of NO_2^- [mg dm^{-3}]
$\mathrm{NO}_{3,\mathrm{in}}$	input concentration of NO_3^- [mg dm^{-3}]
q_{BOD_5}	specific substrate consumption rate for BOD_5 [kg (kg^{-1} s^{-1})]
q_{NH_4}	specific substrate consumption rate for NH_4^+ [kg (kg^{-1} s^{-1})]
q_{NO_2}	specific substrate consumption rate for NO_2^- [kg (kg^{-1} s^{-1})]
q_{DN}	specific denitrification rate [kg kg^{-1}s^{-1}]
$q_{\mathrm{BOD}_{5a}}$	specific substrate consumption rate for adsorbed BOD_5 [kg kg^{-1} s^{-1}]
Re	Reynolds number
τ	mean hydraulic residence time [s, h, d]
$\boldsymbol{\tau}_\mathbf{f}$	time retention constant for laminar layer [s]
$\boldsymbol{\tau}_\mathbf{m}$	time retention constant for electrode membrane [s]
$\boldsymbol{\tau}_\mathbf{g}$	time retention constant for electrolyte gel [s]
V_1	bioreactor volume [dm^3]
$V_{2,n}$	$n \in (1 \ldots 10)$ Volume of one tubular reactor cascade [dm^3]
V_{PFR}	total volume of tubular reactor [dm^3, m^3]
WWTP	waste water treatment plant
X	concentration of active biomass [mg dm^{-3}]
Yo6	oxygen consumption per unit mass of substrate [(kg O_2)(kg BOD_5)$^{-1}$]
$Y1$	theoretical stoichiometric ratio $[(\mathrm{kg\ NO}_2)(\mathrm{kg\ NH}_4^+)^{-1}]$
$Y2$	theoretical stoichiometric ratio $[(\mathrm{kg\ NO}_3^-)(\mathrm{kg\ NO}_2^-)^{-1}]$
$Y3$	theoretical stoichiometric ratio $[(\mathrm{kg\ O}_2)(\mathrm{kg\ NH}_4^+)^{-1}]$
$Y4$	theoretical stoichiometric ratio $[(\mathrm{kg\ O}_2)(\mathrm{kg\ NO}_2^-)^{-1}]$

Costs of wastewater treatment are today an integral part of fees for industrial producers and households. Electricity power needed for the aeration devices (rotary blowers, compressors) is crucial part of operating costs in the wastewater treatment plant. Usually, aeration in the wastewater treatment plant is regulated by dissolved oxygen measurement and appropriate time course program of oxic/anoxic phases. There are two different possible locations appropriate for placement of oxygen electrode:

(i) directly in the fluid medium of bioreactor and
(ii) exit spillway syphon shaft (outlet of bioreactor).

Positioning of the electrode in the shaft has a consequence that information on dissolved oxygen concentration in the aeration tank is time delayed. Delaying time depends on length of syphon shaft and fluid velocity through it.

This raises the question on significance of oxygen electrode position on efficiency of biological processes and electrical consumption, as well as which position is better in that respectively.

The simplest way to address the question above would be to place two oxygen electrodes in the same plant: one directly in the bioreactor fluid, and other one in the outlet shaft. Alternatively, it is possible to perform two consecutive experiments, one with electrode placed in the bioreactor and second one with electrode in the outlet shaft. Unfortunately, some difficulties exist in the solution by the first way because, it is practically impossible to find two identical electrodes with the same response function. Small differences in uniformity of membrane material and gel thickness (on the microscopic level!) are responsible for distinctions in response rate of two electrodes. In addition, there are also influences caused by differences in thickness of (position-dependent!) stagnant fluid layer thickness next to the membrane surface.

The consequence is different for different fluid velocities gradients around electrode on two electrode positions. Oxygen electrode is a master monitoring instrument responsible for regulation of exchange of oxic/anoxic cycles in standard daily aeration procedure. As elaborated above, the position of electrode influences both, the speed electrode response and time delay defined by the flow rate from the well mixed zone in the bioreactor to the position in the syphon shaft.

The accuracy of standard commercially available electrodes is sufficient for the practical control of oxygen concentration in WWTP, but in the same time the slow response to the step changes is insufficient for detailed kinetic investigations. The additional problem is that only one electrode can be the leading instrument for the automatic oxygen control (start of aerators). On the other hand, application of two consecutive experiments (one with electrode placed in the bioreactor and the second one, with electrode in the outlet shaft) is simply a non complete solution because of two reasons:

(I) variations in stagnant layer thickness (caused by flow variability in time) and
(II) variation of water quality in time.

To overcome the experimental obstacles mentioned above, we tried to solve the problem with mathematical modelling. This way practically endless duration of the "experiment" under same conditions is ensured, it is possible to hold the constant "quality" and "flow" of the waste water, and to have two "identical electrodes" with stable and "identical electrode response" on two "positions".

The aim of this work was:

–to find an exact and optimal solution by means of mathematical modelling for position of polarographic oxygen electrodes in the well mixed type of closed loop reactors for waste water treatment,
–to develop and use a suitable computing method for optimization of the electrical power consumption for aeration,
–to detect the consequences of placement of oxygen electrode (the bioreactor or in exit shaft) on the biological process in WWTP.

2. Materials and methods

2.1. Waste water treatment plant

Waste water treatment plant is 96.000 PE (population equivalents) capacity, equipped with aerated sand settler 330 m^3, double prime settler 2×1000 m^3, two closed loop bioreactors well mixed type (2×3400 m^3) with pipe shaped micro-pore aerators on the bottom (Fig. 1), two secondary settlers radial streaming type (2×2210 m^3), sludge recycling and centrifugal sludge dehydration devices. Bioreactors are operating with active sludge recycling and repeating nitrification/de-nitrification cycles (oxic/anoxic phases) controlled by dissolved oxygen concentration in the range 0–2 mg dm^{-3}. Average flow of sewage water was 94 dm^3 s^{-1}, sludge recycling flow was 60 dm^3 s^{-1}.

2.2. Dissolved oxygen measuring

For the dissolved O_2 measurement, polarographic Ag/AgBr oxygen electrode COS 3 (with Au cathode, Teflon membrane, and electrolyte COY3-F, 90% response time = 180 s, 99% response time = 540 s) adapt for the amperometric measurement of output signal by Liquisys COM 250 S 1AB02 device (both from "Endress & Hauser", Germany), was used.

2.3. Analytical methods

COD values of waste water and purified water were determined by ISO 15705:2002 dichromate method. BOD_5 was measured by barometric method using "OXYTOP IS 12" device (WTW, Weinheim, Germany). Nitrates and nitrite were determined by spectrophotometric sulphanil method [5]. Ammonia was determined by nitroprusside method (ISO 7150-1:1998). Suspended solids were determined according to ISO 11923:1997 method.

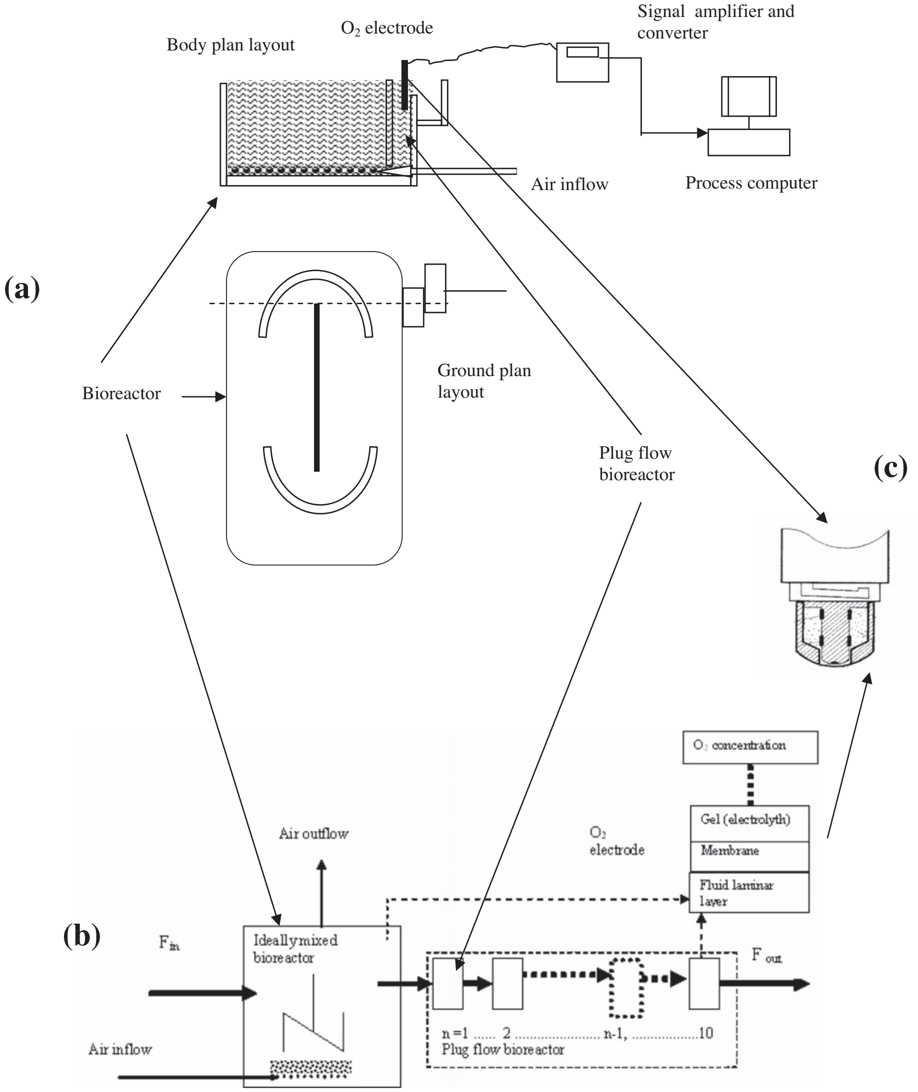

Fig. 1. Simplified schematic structure of the observed system. (a) Ground and body plan layout, (b) model structure, (c) oxygen electrode.

3. Mathematical models

3.1. Oxygen electrode model

The basis for the mathematical model of electrode was an assumption of existence of three oxygen diffusion resistance layers on the oxygen path from the fluid to the cathode [6,7]:

–laminar layer of fluid along the electrode membrane,
–membrane layer and
–electrolyte gel in space between membrane and cathode.

The mathematical model of oxygen electrode was established as the interconnected system of three differential equations:

$$d(C_{\mathrm{f}})/dt = -(C_{\mathrm{f}} - C_{\mathrm{L}})/\tau_{\mathrm{f}} \quad \text{(for the laminar layer)}, \tag{1}$$

$$d(C_{\mathrm{m}})/dt = -(C_{\mathrm{m}} - C_{\mathrm{f}})/\tau_{\mathrm{m}} \quad \text{(for the membrane)}, \tag{2}$$

$$d(C_{\mathrm{g}})/dt = -(C_{\mathrm{g}} - C_{\mathrm{m}})/\tau_{\mathrm{g}} \quad \text{(for the electrolyte gel)}. \tag{3}$$

Model was validated by implementation of ascending and descending step stimulus (Heaviside's function) for oxygen concentration and by comparison of simulated (modelled) electrode response with real experimental responses.

3.2. Mathematical model of process in the bioreactor

Simplified mathematical model of biological process based on ASM-3_2N model [8] was established. The following simplifications were introduced:

- influence of pH was not taken into account, it is assumed as constant for the short time period,
- hydrolysis of complex compounds was neglected, it is assumed that complex compounds are first adsorbed on activated sludge biomass, so hydrolysis rate and consumption rate of such compounds are contained in specific adsorption rate and in specific substrate consumption rate for adsorbed BOD_5,
- ammonification was neglected (it was not experimentally evidenced),
- constant value of the biomass concentration in the bioreactor is assumed (specific death rate and specific growth rate were significantly lower than reaction rates).

Kinetic substrate saturation constants and inhibition rate constants were taken from previous ASM-3 and ASM-3_2N models [8,9], the specific consumption rates were experimentally determined for the examined plant.

Mathematical model for the biological process in the bioreactor was divided in two sub models:

- sub model for the well mixed continuous bioreactor (ideally mixed stirred tank), and
- sub model for the syphon output shaft (represented by continuous plug flow bioreactor)

3.2.1. Sub model structure for the ideally mixed stirred tank

Mathematical model of ideally mixed bioreactor consists of a system of six differential equations related to the biological and hydrodynamic influences.

$$\frac{d(\mathrm{BOD}_5)}{dt} = -r1 + [(F + F_\mathrm{r})/V_1] * \left(\mathrm{BOD}_{5,\mathrm{in}} - \mathrm{BOD}_5\right), \tag{4}$$

$$\frac{d(\mathrm{NH}_4)}{dt} = -r2 + [(F + F_\mathrm{r})/V_1] * \left(\mathrm{NH}_{4,\mathrm{in}} - \mathrm{NH}_4\right), \tag{5}$$

$$\frac{d(\mathrm{NO}_2)}{dt} = Y1 * r2 - r3 + [(F + F_\mathrm{r})/V_1] * \left(\mathrm{NO}_{2,\mathrm{in}} - \mathrm{NO}_2\right), \tag{6}$$

$$\frac{d(\mathrm{NO}_3)}{dt} = Y2 * r3 - r4 + [(F + F_\mathrm{r})/V_1] * (\mathrm{NO}_{3,\mathrm{in}} - \mathrm{NO}_3), \tag{7}$$

$$\frac{d(\mathrm{BPK}_5 a)}{dt} = r1 - r5 - r4 - (F_\mathrm{r}/V1) * \mathrm{BPK}_5 a_n - [(F + F_\mathrm{r})/V_1] * \mathrm{BOD}_{5a}, \tag{8}$$

$$\frac{d(\mathrm{C}b_{\mathrm{O}_2})}{dt} = -Y3 * r2 - Y4 * r3 - \mathrm{Yo6} * r5 + r6 - [(F + F_\mathrm{r})/V_1] * \mathrm{C}b_{\mathrm{O2}}. \tag{9}$$

Kinetic rate equations contained in the right-hand side of above equation system are cited below:

- anaerobic adsorption of BOD_5 on biomass

$$r1 = k_\mathrm{STO} * \frac{\mathrm{BOD}_5}{\mathrm{BOD}_5 + Ks} * \left(1 - \frac{\mathrm{BOD}_5 a}{\mathrm{BOD}_5}\right) * X, \tag{10}$$

- aerobic conversion $NH_4^+ \rightarrow NO_2^-$

$$r2 = q_\mathrm{NH4} * \frac{\mathrm{NH}_4}{\mathrm{NH}_4 + K_{\mathrm{NH}_4}} * \frac{\mathrm{C}_{b\mathrm{O}_2}}{\mathrm{C}_{b\mathrm{O}_2} + Ka_{\mathrm{O}_2}} * X, \tag{11}$$

- aerobic conversion $NO_2^- \rightarrow NO_3^-$

$$r3 = q_\mathrm{NO2} * \frac{\mathrm{NO}_2}{\mathrm{NO}_2 + K_{\mathrm{NO}_2}} * \frac{\mathrm{C}_{b\mathrm{O}_2}}{\mathrm{C}_{b\mathrm{O}_2} + Ka_{\mathrm{O}_2}} * X, \tag{12}$$

- de-nitrification, $NO_3^- \rightarrow N_2$

$$r4 = q_{\mathrm{DN}} * \frac{\mathrm{NO_3}}{\mathrm{NO_3} + K_{\mathrm{NO_3}}} * \frac{\mathrm{BOD_5}a}{\mathrm{BOD_5}a + K_{ads}} * \frac{Ki_{\mathrm{O_2}}}{Ki_{\mathrm{O_2}} + \mathrm{C}b_{\mathrm{O_2}}} * X, \tag{13}$$

–oxidation of adsorbed $\mathrm{BOD_5}$

$$r5 = q_{\mathrm{BOD5a}} * \frac{\mathrm{BOD_5}a}{\mathrm{BOD_5}a + K_{ads}} * \frac{\mathrm{C}b_{\mathrm{O_2}}}{\mathrm{C}b_{\mathrm{O_2}} + Kh_{\mathrm{O_2}}} * X, \tag{14}$$

–oxygen transfer rate

$$r6 = k_{\mathrm{L}}a * \frac{(\mathrm{C}_{\mathrm{O_2},b\max} - \mathrm{C}b_{\mathrm{O_2}}) - (\mathrm{C}_{\mathrm{O_2},t\max} - \mathrm{C}b_{\mathrm{O_2}})}{Ln\left(\frac{\mathrm{C}_{\mathrm{O_2},b\max} - \mathrm{C}b_{\mathrm{O_2}}}{\mathrm{C}_{\mathrm{O_2},t\max} - \mathrm{C}b_{\mathrm{O_2}}}\right)}. \tag{15}$$

3.2.2. Sub model structure for the continuous plug flow bioreactor (syphon output shaft)

Bioreactors output shaft (in reality a rectangular tunnel 5.5 m high, 4 m long and 0.8 m wide (which can be assumed as continuous tubular bioreactor with turbulent flow, Re = 50959) is presented in the sub model as a tank in series of ten ideally mixed compartments (cascade of small bioreactors in the sequence [1] without back-mixing). For each segment (element of cascade) set of six differential equations were placed (Eqs. (16)–(21)), describing the biological processes and hydrodynamic flows and assuming that $k_{\mathrm{L}}a = 0\ \mathrm{s}^{-1}$ (no oxygen enrichment of the wastewater). Volumetric and mass flows from the previous (n-1st) segment represent input flows for the next (nth) segment. Kinetic rate equations ($\mathrm{r}1_n$, $\mathrm{r}2_n$, $\mathrm{r}3_n$, $\mathrm{r}4_n$, $\mathrm{r}5_n$) for each cascade element (1,…,n) are taken from ideal mixed continuous bioreactor model (Eqs. (10)–(15)).

$$\frac{d(\mathrm{BOD_5})_n}{dt} = -r1_n + ((F + F_{\mathrm{r}})/V_{2n}) * (\mathrm{BOD}_{5,n-1} - \mathrm{BOD}_{5,n}), \tag{16}$$

$$\frac{d(\mathrm{NH_4})_n}{dt} = -r2_n + ((F + F_{\mathrm{r}})/V_{2n}) * (\mathrm{NH}_{4,n-1} - \mathrm{NH}_{4,n}), \tag{17}$$

$$\frac{d(\mathrm{NO_2})_n}{dt} = Y1 * r2_n - r3_n + ((F + F_{\mathrm{r}})/V_{2n}) * (\mathrm{NO}_{2,n-1} - NO_{2,n}), \tag{18}$$

$$\frac{d(\mathrm{NO_3})_n}{dt} = Y2 * r3_n - r4_n + ((F + F_{\mathrm{r}})/V_{2n}) * (\mathrm{NO}_{3,n-1} - \mathrm{NO}_{3,n}), \tag{19}$$

$$\frac{d(\mathrm{BOD_5}a)_n}{dt} = r1_n - r5_n - r4_{\mathrm{n}} + ((F + F_{\mathrm{r}})/V_{2n}) * (\mathrm{BOD}_{5a,n-1} - \mathrm{BOD}_{5a,n}), \tag{20}$$

$$\frac{d(\mathrm{C}_{\mathrm{PFR,O_2}})_n}{dt} = -Y3 * r2 - Y4 * r3 - \mathrm{Yo6} * r5 + ((F + F_{\mathrm{r}})/V_{2n}) * (C_{\mathrm{PFR,O2},n-1} - C_{\mathrm{PFR,O2},n}), \tag{21}$$

$$n = 1, \ldots, 10.$$

3.3. Whole system model and mathematical solution

The studied system in reality is made of three subsystems (bioreactor, syphon i.e. overflow output shaft and oxygen electrode).

Mathematical model was structured similarly, and consists of the following three subsystems (Fig. 1):

–model of continuous ideal mixed bioreactor,
–model of syphon overflow output shaft (continuous plug flow bioreactor) and
–model of the measuring instrument (oxygen electrode).

For the numerical solution of equation systems computer program “Berkeley Madonna” version 8.3.11 was used, with integration method Runge–Kutta fourth degree (RK4) with the self regulated step of integration [10]. Used model parameters are listed in Table 1. An integer model validation was performed for oxic and anoxic phase of bioreactor by comparison of experimental time course of $\mathrm{BOD_5}$, $\mathrm{NO_3^-} - \mathrm{N}$, $\mathrm{NH_4^+} - \mathrm{N}$ and dissolved oxygen concentrations, respectively, with corresponding variables calculated by the mathematical model.

Calculated aeration times (model times) were compared with the real time experimental data.

Table 1
List of geometric, hydraulic, chemical, biological and kinetic parameters used in the model.

Parameter	Size	Unit	Explanation	Reference
X	2142	$[\mathrm{mg\,dm^{-3}}]$	Concentration of active biomass	This work
k	$8.025{*}10^{-4}$	$[\mathrm{s^{-1}}]$	k_{L}a for aerobic phase	Technical data- equipment producer
$q_{\mathrm{BOD_5}}$	$1.157{*}10^{-6}$	$[\mathrm{kg\,kg^{-1}\,s^{-1}}]$	Specific substrate consumption rate for $\mathrm{BOD_5}$	This work
$q_{\mathrm{NH_4}}$	$2.118{*}10^{-6}$	$[\mathrm{kg\,kg^{-1}\,s^{-1}}]$	Specific substrate consumption rate for $\mathrm{NH_4^-}$	This work
$q_{\mathrm{NO_2}}$	$2.824{*}10^{-6}$	$[\mathrm{kg\,kg^{-1}\,s^{-1}}]$	Specific substrate consumption rate for $\mathrm{NO_2^-}$	This work
q_{DN}	$6{*}10^{-7}$	$[\mathrm{kg\,kg^{-1}\,s^{-1}}]$	Specific de-nitrification rate	This work
$q_{\mathrm{BOD_5}a}$	$1.35{*}10^{-6}$	$[\mathrm{kg\,kg^{-1}\,s^{-1}}]$	Specific substrate consumption rate for adsorbed $\mathrm{BOD_5}$	This work
k_{STO}	$6.57{*}10^{-6}$	$[\mathrm{kg\,kg^{-1}\,s^{-1}}]$	Specific adsorption rate for $\mathrm{BOD_5}$	[9]
Ks	3	$[\mathrm{mg\,dm^{-3}}]$	Saturation constant for $\mathrm{BOD_5}$	[9]
$\mathrm{KaO_2}$	0.5	$[\mathrm{mg\,dm^{-3}}]$	Saturation constant for $\mathrm{O_2}$, for autotrophic biomass	[9]
$\mathrm{KhO_2}$	0.1	$[\mathrm{mg\,dm^{-3}}]$	Saturation constant for $\mathrm{O_2}$, for heterotrophic biomass	[9]
K_{NH_4}	2	$[\mathrm{mg\,dm^{-3}}]$	Saturation constant for $\mathrm{NH_4^-}$	[9]
K_{NO_2}	0.5	$[\mathrm{mg\,dm^{-3}}]$	Saturation constant for $\mathrm{NO_2^-}$	[9]
K_{NO_3}	0.5	$[\mathrm{mg\,dm^{-3}}]$	Saturation constant for $\mathrm{NO_3^-}$	[9]
K_{ads}	1	$[\mathrm{mg\,mg^{-1}\,dm^{-3}}]$	Saturation constant for adsorbed $\mathrm{BOD_5}$	[9]
$Ki\mathrm{O_2}$	0.5	$[\mathrm{mg\,dm^{-3}}]$	Inhibition constant for $\mathrm{O_2}$	[9]
$C(\mathrm{O_2})_{,\mathrm{bmax}}$	13.29	$[\mathrm{mg\,dm^{-3}}]$	Saturation constant for $\mathrm{O_2}$ in wastewater on bottom of the bioreactor	
$C(\mathrm{O_2})_{,\mathrm{tmax}}$	8.6	[mg dm–3]	Saturation constant for $\mathrm{O_2}$ in wastewater on top of the bioreactor	
Yo6	1.3	$[(\mathrm{kg\,O_2})(\mathrm{kg\,BOD_5})^{-1}]$	Oxygen consumption per unit mass of substrate	[18]
$Y1$	2.5556	$[(\mathrm{kg\,NO_2^-})(\mathrm{kg\,NH_4^+})^{-1}]$	Theoretical stoichiometric ratio	This work
$Y2$	1.3478	$[(\mathrm{kg\,NO_3^-})(\mathrm{kg\,NO_2^-})^{-1}]$	Theoretical stoichiometric ratio	This work
$Y3$	2.666	$[(\mathrm{kg\,O_2})(\mathrm{kg\,NH_4^+})^{-1}]$	Theoretical stoichiometric ratio	This work
$Y4$	0.3478	$[(\mathrm{kg\,O_2})(\mathrm{kg\,NO_2^-})^{-1}]$	Theoretical stoichiometric ratio	This work
Geometric and hydraulic parameters of the wastewater treatment plant used in the mathematical models				
F	94	$[\mathrm{dm^3\,s^{-1}}]$	Waste water flow	
F_{r}	60	$[\mathrm{dm^3\,s^{-1}}]$	Recirculation flow	
V_1	6800000	$[\mathrm{dm^3}]$	Bioreactor volume	
V_{PFR}	17600	$[\mathrm{dm^3}]$	Total volume of tubular reactor	
$V_{2,n}\ n \in (1\ldots10)$	1760	$[\mathrm{dm^3}]$	Volume of one tubular reactor cascade	
Input parameters of the wastewater treatment plant used in the mathematical models				
$\mathrm{BOD_{5,in}}$	190	$[\mathrm{mg\,dm^{-3}}]$	Input concentration of $\mathrm{BOD_5}$	This work
$\mathrm{NH_{4in}^+}$	12	$[\mathrm{mg\,dm^{-3}}]$	Input concentration of $\mathrm{NH_4^+}$	This work
$\mathrm{NO_{2,in}^-}$	0	$[\mathrm{mg\,dm^{-3}}]$	Input concentration of $\mathrm{NO_2^+}$	This work
$\mathrm{NO_{3,in}^+}$	3	$[\mathrm{mg\,dm^{-3}}]$	Input concentration of $\mathrm{NO_3^+}$	This work
$\mathrm{BOD_{5,amax}}$	10	$[\mathrm{mg\,dm^{-3}}]$	Maximum possible amount of adsorbed $\mathrm{BOD_5}$ calculated from the weight of the biomass	This work

4. Results and discussion

4.1. Validation of oxygen electrode model

The polarographic oxygen electrode is a typical instrument with relatively long delayed response to the step size change of measured variable. It is known that the rates of biochemical reactions in the biomass are kinetically faster than the response of the $\mathrm{O_2}$-electrode. In the tested plant, residence time of fluid stream through shaft was 228 s, and the 90% response of electrode was practically the same order of magnitude (180 s). That is why it was necessary to include the electrode response in the kinetic system and why the related sub model must be included in the whole model system. Because of additional electrochemical reactions with water ingredients on the cathode, an application of “naked” oxygen electrode (without membrane and electrolyte gel) was not the right solution for our experiments. Another suitable method which can be applied for measurement of dissolved oxygen is the luminescent dissolved oxygen measurement. This method offers shorter response times and it is not sensitive to the side reactions [11–14]. Unfortunately, it is more of scientific significance and still rarely applied in waste water treatment plants as regulating device for oxygen concentration control.

During standard operational period there are alternating changes of oxic/anoxic phases in the WWTP (the rise up and fall down of dissolved oxygen concentration in the bioreactor fluid). For that reason, we have tested both electrode responses: on the ascending and on the descending step stimulus. The results are presented on Fig. 2.

As seen in Fig. 2, change of $\mathrm{O_2}$ concentration obtained by model is in very good agreement with experimental electrode response to the ascending as well to the descending step stimulus. However different values of model parameters (τ_f, τ_i, τ_g)

were found for ascending and descending response to the stimulus. This is especially emphasised (by two orders of magnitude) in the case of time retention constant for laminar layer (τ_f). The reason for that could be that in the case of ascending stimulus an oxygen gradient has a negative value through the whole system (fluid layer, membrane, gel, cathode) with maximal concentration of oxygen in the fluid layer and with minimal concentration by the cathode surface). In contrary, if descending stimulus is applied, the electrode system is saturated with oxygen on the beginning of experiment. After the transferring of electrode in the "oxygen zero" solution, oxygen gradients are bidirectional (low concentration in the fluid layer, high concentration in the membrane and gel, as well as low concentration by the cathode.

These two situations can not be modelled with the same set of parameters. For modelling of oxygen electrode two possibilities are available:

–to estimate the mathematical transfer function
–to develop a physical model

In our experiments the target of the work was not the oxygen electrode and response itself. The problem of electrode was included only because of its significant influence on the final results achieved by different positioning of electrode. Therefore for the modelling of electrode (for the whole examined period of oxygen concentration change, aeration and anoxic part of cycle) we have applied diffusion resistance model with the set of three parameters (τ_f, τ_l and τ_g), described earlier [15]. Parameters for simulation were achieved from descending stimulus experiment. This can be done because the oxygen concentration change in the whole cycle fall into low dissolved oxygen concentration range (0–2 mg/dm^3 and 0–3 mg/dm^3). In this range a good agreement between model and experiment was achieved if the set of descending response parameters was applied. The control experiment presented on Fig. 2(c) (for the ascending and descending part of oxygen concentration curve) confirmed this approach.

During testing of the model sensitivity by positive and negative variation of parameters the least impact on simulated result was detected for parameter τ_g (related to the electrolyte gel). Values of the other two parameters τ_f and τ_m have a greater impact on the result (results not shown). Mathematical simulation was conducted with chosen optimal values of model parameters so the satisfied result of modelled electrode response was achieved (Fig. 2(c)). In addition, above approach is applicable only on polarographic oxygen electrodes with relatively thick robust membranes and with gel-electrolyte covered cathode. For other types of electrodes an appropriate model adaptation will be probably needed.

4.2. Model structure, testing and sensitivity of the waste water treatment model

Each of two bioreactors (2 × 3400 m^3) was loaded with 47 dm^3 s^{-1} of waste water and 30 dm^3 s^{-1} of recycled sludge originated from secondary settler. Therefore it can be characterised with mean residence time τ = 12,26 h and with dilution rate D = 0.081 h^{-1}. Based on the construction of bioreactor which was closed loop well mixed type, it has been possible to choose between three types of model approaches:

(i) closed loop tank in series with or without back-mixing,
(ii) axial dispersion model and
(iii) ideally mixed tank model.

In this work ideally mixed tank model was chosen based on results of De Clercq et al. [4] where it was proven that, in the case of long residence times, the 65% of bioreactor volume could be represented by one ideally mixed tank.

Second part of the biological system the syphon outlet shaft was characterised by turbulent flow regime (Re = 50959) and by relatively short residence time (τ = 228 s). According to previously published results of Potier et al. [16] for full scale and bench scale plants, such case would need more than twenty well mixed cells in cascade for the successful modelling. In the same time it is very well known that flows with high Reynolds number can be approached as "close to piston" flows (similar to pipe shaped holding sections of continuous sterilization devices). Re-number in this plant-shaft was over 50000, so the tank in series approach was chosen. Because of results of Potier et al. [16] it was necessary to test the number of cells in the model. Results of this testing are presented on Figs. 3 and 4. Based on these results, thank in series model with ten cells was chosen as potentially satisfactory.

According to mathematical modelling theory [17,2,3] the sensitivity of mathematical models for bio systems to the change of parameters should be stringently and completely tested. In the real system, the specific rate of substrate consumption ($q\text{BOD}_{5,a}$), the flow of waste water (as one of the factors that determines the load) and oxygen consumption per unit mass of substrate (Yo6) have significant influence on the aeration time. That is why the cited parameters and variables were tested. As criterion for the goodness of influence of model parameters, the duration of aeration cycle (oxic phase) was chosen. The results of model sensitivity to the parameters variations are presented in Fig. 5.

Results in Fig. 5 show that the specific substrate consumption rate ($q\text{BOD}_{5,a}$) and oxygen consumption per unit mass of substrate (Yo6) have the greatest impact on the modelled oxic phase duration (aeration time) for both electrode positions. Simulated aeration time has been less influenced by the inflow of wastewater than by other two parameters (Yo6, $q\text{BOD}_{5,a}$), because of slow system response caused by relatively high residence time usually applied in the waste water treatment plants. In addition, Fig. 5 shows that there is an obvious difference in the simulated aeration time (depending on two posi-

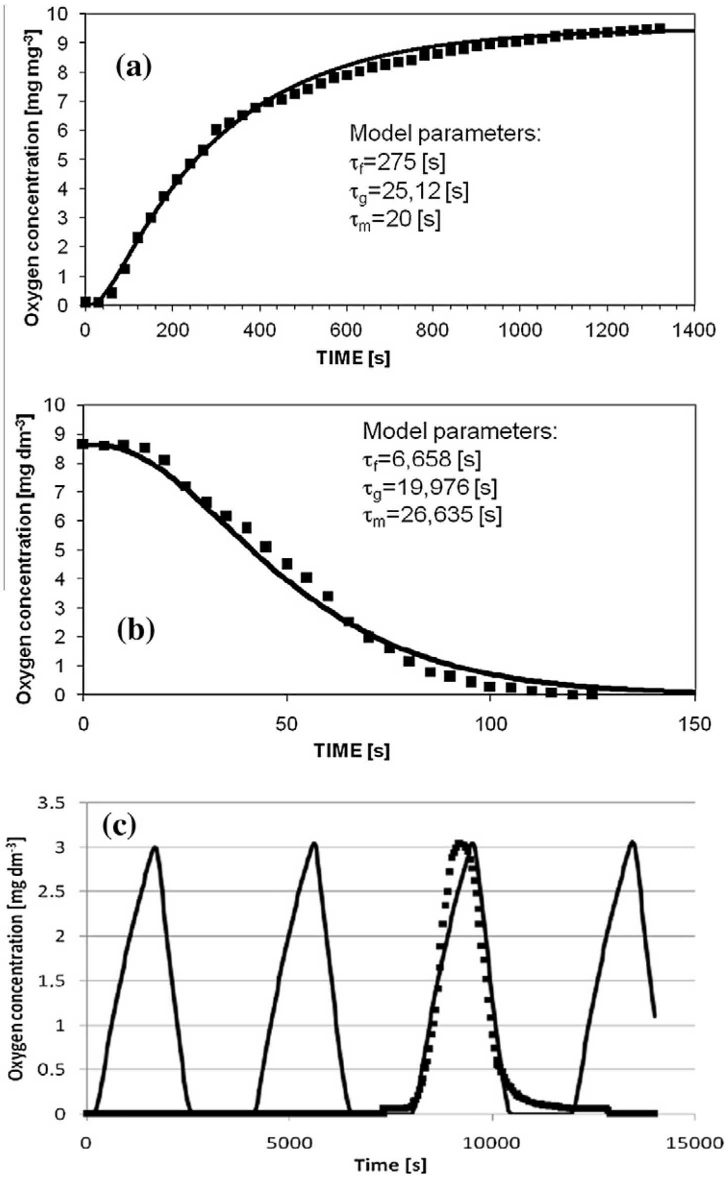

Fig. 2. Oxygen electrode response for ascending (a) and descending, (b) changes of dissolved oxygen. Comparation between values for experimental oxygen concentration change and oxygen concentration obtained by mathematical model, and (c) (■ measured values of dissolved oxygen; ■ modelled values of dissolved O_2).

tions of oxygen electrode tested). If all three reference values of parameters and bioreactor position of electrode were applied, 668 seconds of aeration time was necessary to reach modelled dissolved oxygen concentration of 2 mg dm^{-3}. In contrary, when electrode was modelled in the outlet shaft, 1023 s were required to reach the same concentration. This difference is dependent on the degree of parameter altering and on the direction (positive/negative) of change, but it is significant in the whole range of testing (±20% of reference value).

4.3. Results obtained from model simulation

After testing of sub models sensitivity to the parameters variation, the real situation was simulated using the whole mathematical model with all three sub models included. Related results are presented in Fig. 6.

Simulated results presented in Fig. 6 were compared with the shape and the magnitude (maximum/minimum) of analytical results obtained in the laboratory. The time course of oxygen concentration was compared with plant oxygen monitoring system. Simulated and measured results are in good agreement (Fig. 6, Table 2), thus the developed model was accepted as a good tool for the further work.

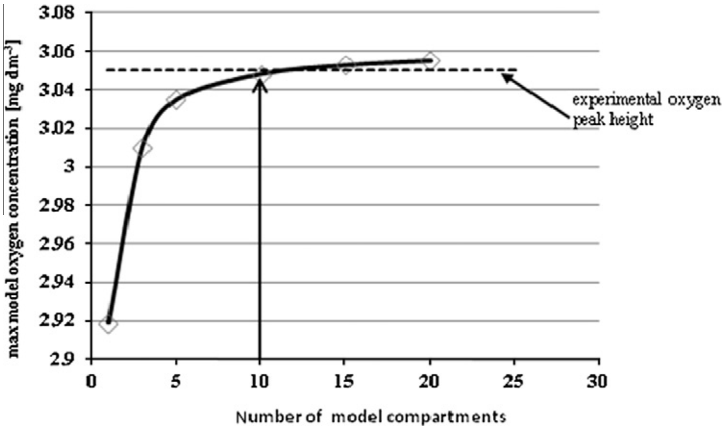

Fig. 3. Dependency of maximum modelled oxygen concentration by number of cascade cells in cascade plug flow bioreactor (◇ modelled values, ● maximum oxygen concentration, experimental value).

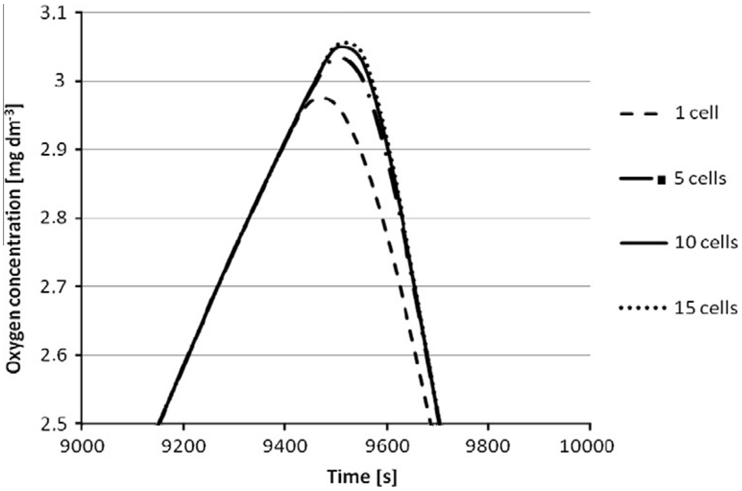

Fig. 4. Difference in maximum modelled oxygen concentration for different number of cascade cells.

Using full tested model and optimised reference parameters, the whole system was simulated. In this new simulation, focal point was the oxygen electrode position. Results of simulation are presented on Figs. 7 and 8 as well as in the Table 3

Results in Fig. 7, show that there is a difference between two tested positions of electrode. It is possible to see (Table 3) that the total operating time of the air compressors is significantly shortened for the simulated electrode in the bioreactor position, if compared with simulation of electrode in the outlet shaft place (7.9–8.41 h d^{-1}). At the same time, the duration of a working cycle falls from 891 s (for the shaft position) to 652 s (bioreactor position). However, the simulated positioning of electrode in the bioreactor caused a negative phenomenon since it leads to a greater number of aeration cycles per day (43.6 cycles per day for bioreactor position and 34 cycles per day for the output shaft position). That means the number of start-ups and shut-downs of the air compressors will be raised up in a day if the oxygen electrode will be positioned in the bioreactor. Unfortunately, this fact resulted in greater exposure of electromechanical equipment (motors and switchers) to transient electrical currents phenomena. To eliminate above mentioned negative effects on electrical equipment, higher oxygen concentration (3 mg dm^{-3}) as the shutdown point for compressors was simulated (Fig. 8).

Although, as it is very well known how the increased oxygen concentration in the bioreactor influences waste water treatment, there are less reports about combined impact of oxygen electrode response and prolonged oxic phase.

The outcome results (Fig. 8, Table 3) have shown that the total compressor operating time is also shorter for the bioreactor position than for the shaft position of oxygen electrode (8.73–9.2 h per day). In the same time, the duration of a working cycle is shorter for the bioreactor than for the shaft position (3116–3895 s), respectively. Additionally, the turning off point of compressors at 3 mg dm^{-3} of DO, has a further negative impact: the number of cycles in that case has risen up from 22.2 cycles per day -shaft position to 27.7 cycles per day -bioreactor position. All together, if compared with results corresponding to the 2 mg dm^{-3} aeration breakpoint, the physiologically unnecessary high aeration break point at 3 mg dm^{-3} has

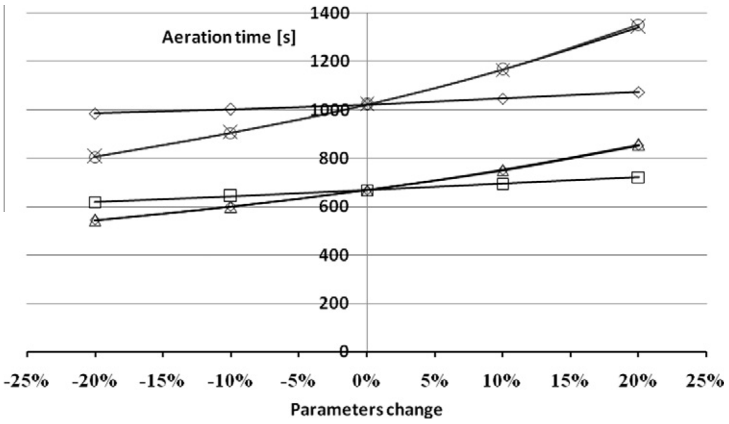

Fig. 5. The influence of variation of model parameters on the aeration time (**$qBOD_{5a}$** Specific consumption rate of adsorbed BOD_5, △ electrode measuring in bioreactor, ○ electrode in shaft; **Yo6** Oxygen consumption per unit mass of substrate, □ electrode measuring in bioreactor, × electrode measuring in shaft; **F** Flow of waste water, ◇ electrode measuring in bioreactor × electrode measuring in shaft).

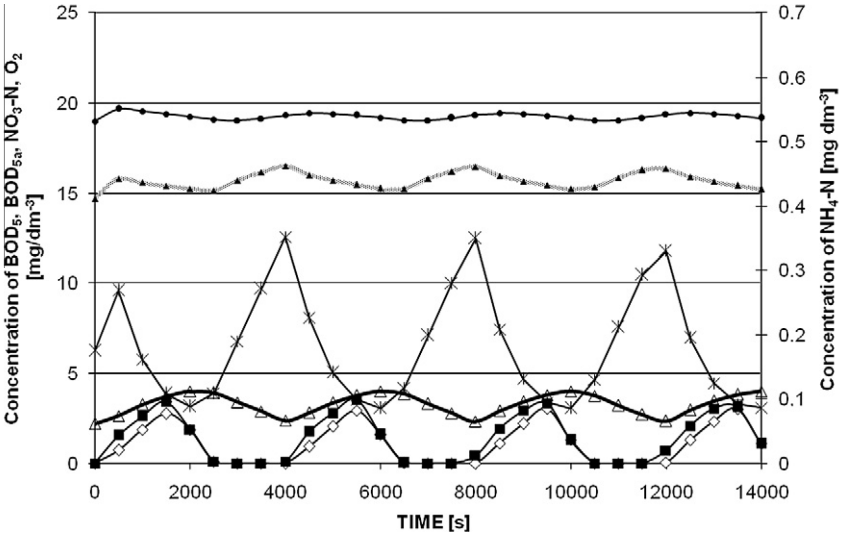

Fig. 6. Time course of BOD_5 (●), BOD_{5a} (▲), $NH_4^- - N$ (★), $NO_3^- - N$ (△) concentrations, and O_2 concentration in bioreactor (■) and plug flow reactor (◇), achieved by mathematical simulation.

Table 2
Average values of concentration of BOD_5, $NH_4^+ - N$ and $NO_3^+ - N$ calculated in the model and compared with laboratory values achieved by 24 h testing.

	Average concentration [mg dm^{-3}] (model)	Measured concentration [mg dm^{-3}] (experiment)
BOD_5	19.24	19.0
NH_4-N	0.184	0.3
NO_3-N	3.302	2.9

caused a longer aeration time, longer working cycle and greater total working time of compressors. In the same time at these conditions, number of working cycles per day have been reduced (Table 3).

5. Conclusions

Mathematical modelling of waste water treatment system using three sub models (for oxygen electrode, ideally mixed stirred tank bioreactor and plug flow reactor) is a suitable tool for the optimisation of aeration process in WWTP if closed

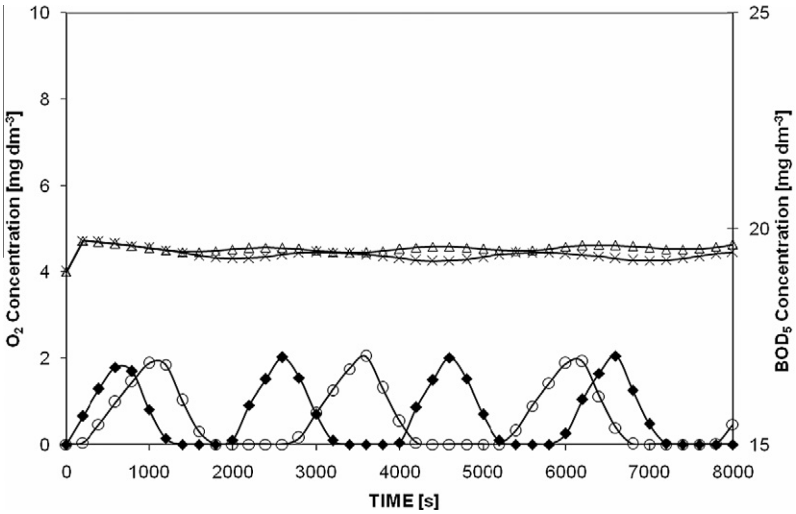

Fig. 7. The time course of simulated BOD$_5$ (△ O$_2$ electrode in bioreactor, ★ electrode in shaft) and dissolved oxygen concentration (♦ electrode in bioreactor, ○ electrode in shaft) values for two positions of the electrode at 2 mg dm^{-3} O$_2$ as the breakpoints for aeration.

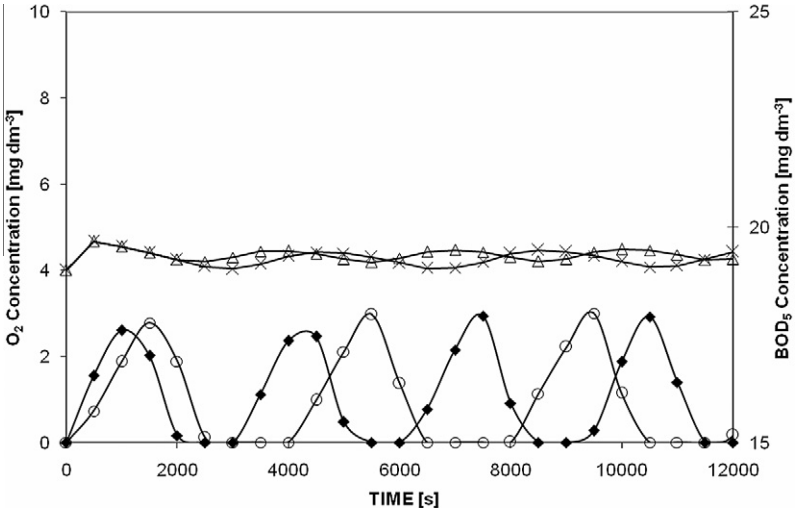

Fig. 8. The time course of simulated BOD$_5$ (△ O$_2$ electrode in bioreactor, ★ electrode in shaft) and dissolved oxygen concentration (♦ electrode in bioreactor, ○ electrode in shaft) values for two positions of the electrode at 3 mg dm^{-3} O$_2$ as the breakpoints for aeration.

Table 3
Summarized simulated results for aeration time, working cycle time, number of working cycles daily and working time of compressors per day.

Aeration degree	2 mg O$_2$ dm^{-3}		3 mg O$_2$ dm^{-3}	
Electrode position	Bioreactor	Exit shaft	Bioreactor	Exit shaft
Aeration time per cycle [s]	652	891.33	1135.3	1494.33
Duration time of working cycle (aerobic and anaerobic phase) [s]	1982.5	2542.5	3116.3	3895
Number of working cycles in one day [d^{-1}]	43.58	33.98	27.725	22.182
Total working time of compressors [h d^{-1}]	7.89	8.414	8.735	9.207

loop well mixed type of bioreactors are installed and if polarographic oxygen electrode with thick membrane and gel layer is in use. This method is successful for testing of oxygen electrode position impact on process efficiency.

According to simulated results, position of the oxygen electrode in the bioreactor (instead in the bioreactors outlet shaft) cause the shortening of working cycle 13%, the reduction of daily working time of compressors for 0.5 h and increase of number of oxic/anoxic cycles per day by 29%.

If compared with results corresponding to the dissolved oxygen breakpoint of 2 mg dm^{-3} (aeration cut off point), an increase of breakpoint to 3 mg/dm^{-3} causes a longer aeration time, longer working cycle time, greater total working time of compressors and lower number of working cycles per day.

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